

Supporting Information

A putative prophylactic solution for COVID-19: Development of multiepitope vaccine candidate against SARS-COV-2 by comprehensive immunoinformatic and molecular modeling approach

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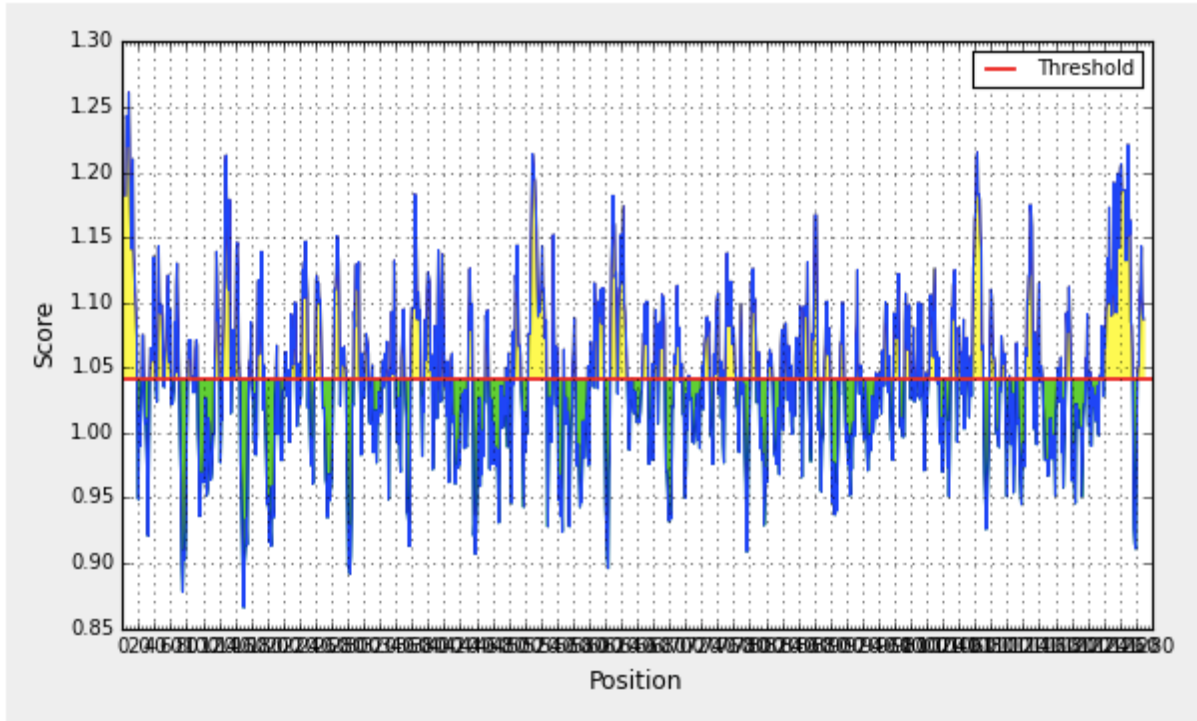


Figure S1: Graphical representation of predicted antigenic propensity of SARS-CoV-2 Spike protein

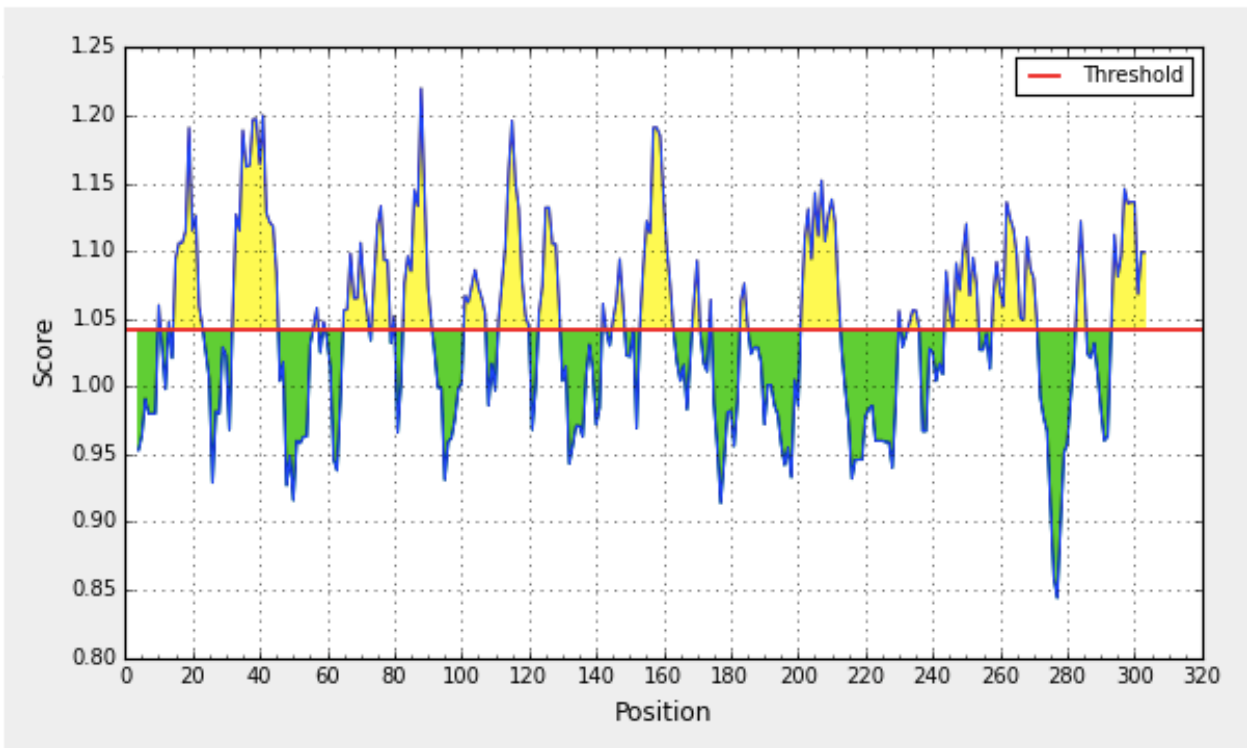


Figure S2: Graphical representation of predicted antigenic propensity of SARS-CoV-2 Main protease

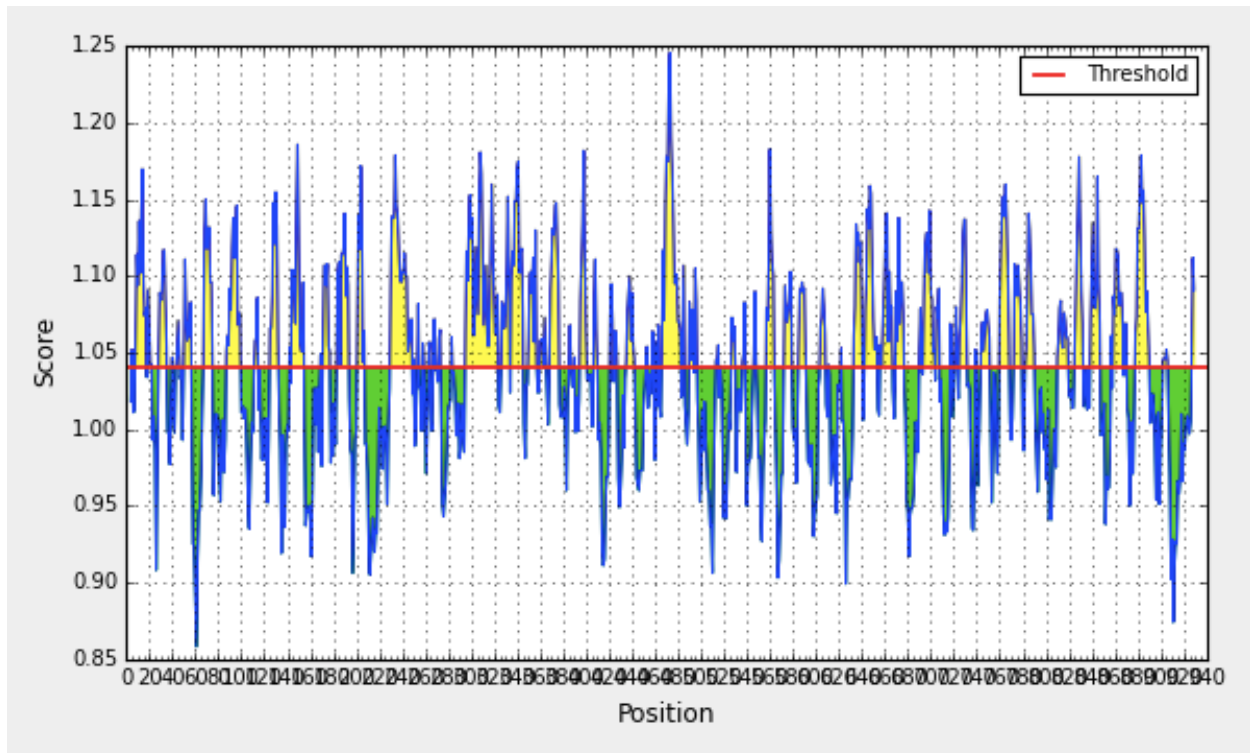


Figure S3: Graphical representation of predicted antigenic propensity of SARS-CoV-2 Nsp12 RNA-dependent-RNA-polymerase (RdRp)

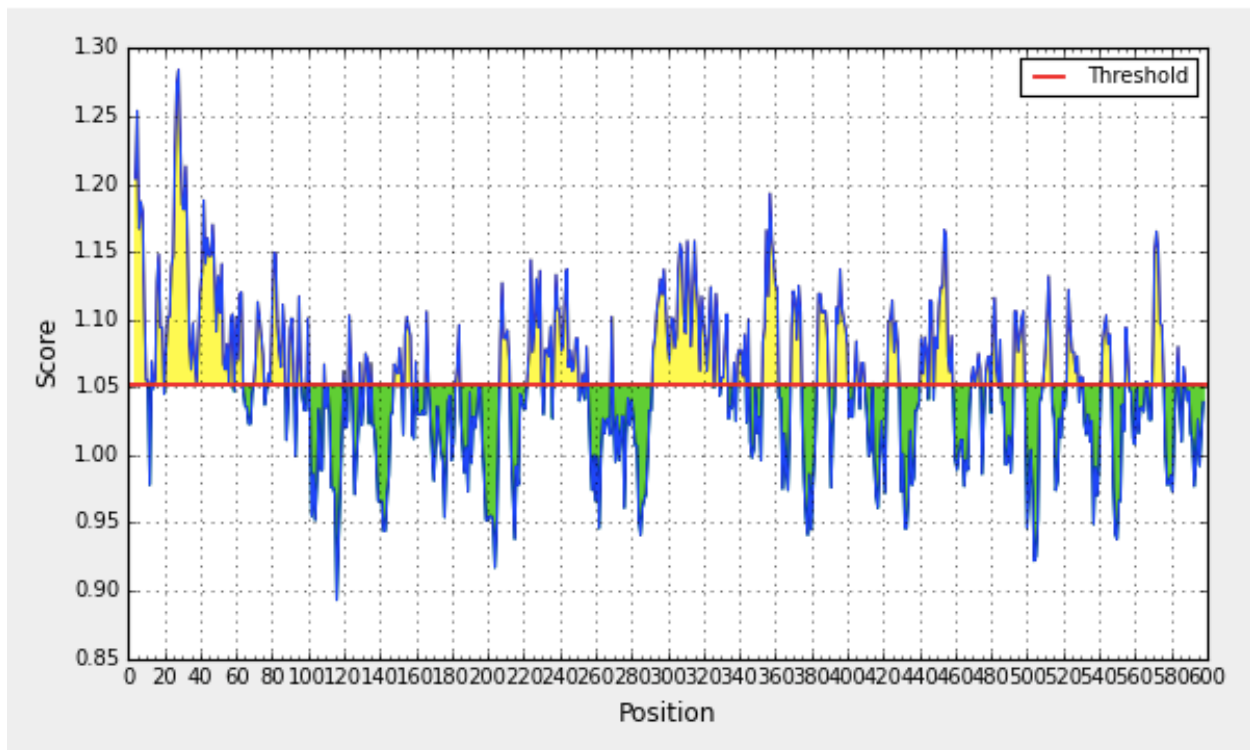


Figure S4: Graphical representation of predicted antigenic propensity of SARS-CoV-2 Nsp13 helicase

GIGDPVTCLKSGAICHVPFCPRRYKQIGTCGLPGTKCCKKP EAAK CVADYSVLYAAYCNDPFLGVY AAY
 MTSCCSCLKAAYSTQDLFLPFAAYTSNQVAVLYAAYKTSVDCTMYAAYVASQSIIAYAAYGAAAYVGY AAY
 RISNCVADYAAYITDAVDCAL AAYECSNLLLQY AAYTVNVLAWLYAAYQTFSLACYAAY
 DYDCVSFCYAAYTANPKTPKYAAYDTDFVNEFY AAYLSFKELLVY AAYSTDVVYRAFAAYFVSLAIDAYAAY
 MVMCGGSLYAAYLSDDAVVCF AAYTTAYANSVFAAYAVVCFNSTYAAYMCDIRQLLFAAYVVDSYYSLLAAY
 VTANVNALLAAYMLVKQGDDYAAYGDDYVYLPYAAYDVHFLYLQYAAYEYADVFLYAAYGVPVVD SYAA
 YSVELKHFFFAAYFVDGVPFVVAAYCCSLSHRFY AAYVTDVTQLYL AAYDVTDVTQLYAAYSSQGSEYDY
 AAYPTLVPQEHYAAYIVDVSALVAAYCIMS DRDLYAAYKVNSTLEQYAAYHYVRITGLYAAYANGQVFGLYA
 AYGSEYDYVIFGPGPGVVVLSFELLHAPATVCGPK GPGPGITGRLQSLQTYVTQQLIRAAEIRGPGPG
 AAYVGYLQPRTFLLKYN GPGPGTGRLQSLQTYVTQQL GPGPGI IAYTMSLGAENSVAYGPGPGGWTFGAGA
 ALQIPFAGPGPGTPKYKFVRIQPGQTFSVLAGPGPGSHNFLVQAGNVQLRVIGGPGPGFVRIQPGQTFSVLA
 CGPGPGPEFYEAMYTPHTVLQ GPGPGSLSHRFYRLANCAQVLS EPGPGPGQKLLKSIAATR GATV GPGPGW
 EPEFYEAMYTPHTVL GPGPGQFHQKLLKSIAATRGA GPGPGKLLKSIAATR GATVV GPGPGMPNMLRIMAS
 LVLARKGPGPGAVASKILGLPTQTVDSSQ GPGPGMQYSTLQGPPTGKS GPGPGETFKLSYGIATVREVLG
 PGPGVGDYFVLTSHTVMPLS GPGPGISPYN SQNAVASKIL EAAK GIINTLQKY YCRVRGGRC AVL SCLPKEE
 QIGKCSTRGRKCCRKK

Figure S5: Multiepitope vaccine construct.

Note: Grey highlighted in start is human β -Defensins hBD-2 (PDB ID: 1FD3) and in the end human β -Defensins hBD-3 (PDB ID: 1KJ6). Yellow color represents CTL epitope while sea green color represents HTL epitope. The linker used are highlight red for 'AAY' and magenta for 'GPGPG'. First 11 yellow peptides belong to SARS-CoV-2 spike protein till **ECSNLLLQY**, next 4 peptide belong to Mpro till **TANPKTPKY**, next 19 peptides from RdRp till **CCSLSHRFY** followed by next 10 peptides from helicase till **GSEYDYVIF**. For HTL, First 6 sea green peptides belong to spike protein till **GWTFGAGAALQIPFA**, next 3 from Mpro till **FVRIQPGQTFSVLAC**, next 8 from RdRp till **AVASKILGLPTQTVDSSQ** followed by last 4 from helicase till **SPYNSQNAVASKIL**.

Table S1: HTL epitope of SARS-CoV-2 Main protease (Mpro) protein having strong binding affinity, predicted by NetMHC-II

Alleles	Peptides	core Oflog50k (aff)	Binding level
DRB1_0101	KYKFVRIQPGQTFSV	0.9145	Strong binder
DRB1_0101	PKYKFVRIQPGQTFS	0.9009	Strong binder
DRB1_0101	YKFVRIQPGQTFSVL	0.9002	Strong binder
DRB1_0101	KFVRIQPGQTFSVLA	0.8791	Strong binder
DRB1_0101	TPKYKFVRIQPGQTF	0.8786	Strong binder
DRB1_0101	NHNFLVQAGNVQLRV	0.8528	Strong binder
DRB1_0101	HNFLVQAGNVQLRVI	0.8521	Strong binder
DRB1_0101	NFLVQAGNVQLRVIG	0.8299	Strong binder
DRB1_0101	SNHNFLVQAGNVQLR	0.8266	Strong binder
DRB1_0101	FVRIQPGQTFSVLAC	0.8181	Strong binder

Table S2: HTL epitope of SARS-CoV-2 RNA polymerase protein having strong binding affinity, predicted by NetMHC-II

Alleles	peptides	core Of log50k (aff)	Binding level
DRB1_0101	PEFYEAMYPHTVLQ	0.9077	Strong binder
DRB1_0101	SHRFYRLANECAQVL	0.9061	Strong binder
DRB1_0101	QKLLKSIAATRQATV	0.9055	Strong binder
DRB1_0101	HQKLLKSIAATRQAT	0.9041	Strong binder
DRB1_0101	HRFYRLANECAQVLS	0.9013	Strong binder
DRB1_0101	EPEFYEAMYPHTVL	0.8989	Strong binder
DRB1_0101	FHQKLLKSIAATRGA	0.8974	Strong binder
DRB1_0101	LSHRFYRLANECAQV	0.8856	Strong binder
DRB1_0101	RFYRLANECAQVLSE	0.8856	Strong binder
DRB1_0101	KLLKSIAATRQATVV	0.8813	Strong binder
DRB1_0101	QFHQKLLKSIAATRQ	0.8702	Strong binder
DRB1_0101	WEPEFYEAMYPHTV	0.8643	Strong binder
DRB1_0101	PNMLRIMASLVLARK	0.8643	Strong binder
DRB1_0101	MPNMLRIMASLVLAR	0.8616	Strong binder
DRB1_0101	SLSHRFYRLANECAQ	0.8596	Strong binder
DRB1_0101	NMLRIMASLVLARKH	0.8539	Strong binder
DRB1_0101	RQFHQKLLKSIAATR	0.8511	Strong binder
DRB1_0101	AMPNMLRIMASLVLA	0.8347	Strong binder
DRB1_0101	LLKSIAATRQATTVI	0.8272	Strong binder
DRB1_0101	MLRIMASLVLARKHT	0.8255	Strong binder
DRB1_0101	FLNRVCGVSAARLTP	0.8249	Strong binder
DRB1_0101	LLVYAADPAMHAASG	0.8236	Strong binder
DRB1_0101	KGFFKEGSSVELKHF	0.8227	Strong binder
DRB1_0101	NRQFHQKLLKSIAAT	0.8223	Strong binder
DRB1_0101	FYAYLRKHFSMMILS	0.8205	Strong binder
DRB1_0101	SFLNRVCGVSAARLT	0.8204	Strong binder
DRB1_0101	FYRLANECAQVLSEM	0.8181	Strong binder
DRB1_0101	ELLVYAADPAMHAAS	0.8163	Strong binder
DRB1_0101	EFYAYLRKHFSMMIL	0.8135	Strong binder
DRB1_0101	LTGHMLDMYSVMLTN	0.8101	Strong binder
DRB1_0101	PDILRVYANLGERVR	0.8087	Strong binder
DRB1_0101	SKGFFKEGSSVELKH	0.8058	Strong binder
DRB1_0101	NPDILRVYANLGERV	0.8054	Strong binder
DRB1_0101	LNRVCGVSAARLTPC	0.8036	Strong binder
DRB1_0101	CSLSHRFYRLANECA	0.8035	Strong binder
DRB1_0101	TGHMLDMYSVMLTND	0.8028	Strong binder

Table S3: HTL epitope of SARS-CoV-2 Nsp13 helicase having strong binding affinity, predicted by NetMHC-II

Alleles	peptides	core Of log50k (aff)	Binding level
DRB1_0101	ASKILGLPTQTVDS	0.8936	Strong binder
DRB1_0101	VASKILGLPTQTVDS	0.8853	Strong binder
DRB1_0101	SKILGLPTQTVDSQ	0.8782	Strong binder
DRB1_0101	MQKYSTLQGPPGTGK	0.8687	Strong binder
DRB1_0101	AVASKILGLPTQTV	0.8627	Strong binder
DRB1_0101	QKYSTLQGPPGTGKS	0.8584	Strong binder
DRB1_0101	TFKLSYGIATVREVL	0.8549	Strong binder
DRB1_0101	VGDYFVLTSHTVMPL	0.8535	Strong binder
DRB1_0101	GDYFVLTSHTVMPLS	0.8510	Strong binder
DRB1_0101	ISPYNSQNAVASKIL	0.8488	Strong binder
DRB1_0101	ETFKLSYGIATVREV	0.8459	Strong binder
DRB1_0101	GMQKYSTLQGPPGTG	0.8449	Strong binder
DRB1_0101	EETFKLSYGIATVRE	0.8418	Strong binder
DRB1_0101	KSHFAIGLALYYPSA	0.8413	Strong binder
DRB1_0101	FKLSYGIATVREVL	0.8376	Strong binder
DRB1_0101	TEETFKLSYGIATVR	0.8363	Strong binder
DRB1_0101	GKSHFAIGLALYYPS	0.8354	Strong binder
DRB1_0101	SPYNSQNAVASKILG	0.8335	Strong binder
DRB1_0101	NVGDYFVLTSHTVM	0.8331	Strong binder
DRB1_0101	DYFVLTSHTVMPLSA	0.8320	Strong binder
DRB1_0101	KYSTLQGPPGTGKSH	0.8313	Strong binder
DRB1_0101	KILGLPTQTVDSQ	0.8259	Strong binder
DRB1_0101	LNVDYFVLTSHTVM	0.8224	Strong binder
DRB1_0101	FISPYNSQNAVASKI	0.8224	Strong binder
DRB1_0101	TGKSHFAIGLALYY	0.8223	Strong binder
DRB1_0101	VGMQKYSTLQGPPGT	0.8146	Strong binder
DRB1_0101	GTGKSHFAIGLALYY	0.8133	Strong binder
DRB1_0101	NAVASKILGLPTQTV	0.8111	Strong binder

Table S3: HTL epitope of SARS-CoV-2 Spike protein having strong binding affinity, predicted by NetMHC-II

alleles	peptides	core Of log50k (aff)	Level of binding
DRB1_0101	VLSFELLHAPATVCG	0.9082	Strong binder
DRB1_0101	LSFELLHAPATVCGP	0.9033	Strong binder
DRB1_0101	VVLSFELLHAPATVC	0.9010	Strong binder
DRB1_0101	SFELLHAPATVCGPK	0.8909	Strong binder
DRB1_0101	VVLSFELLHAPATV	0.8905	Strong binder
DRB1_0101	LQTYVTQQLIRAAEI	0.8745	Strong binder
DRB1_0101	YVGYLQPRTFLLKY	0.8736	Strong binder
DRB1_0101	YVGYLQPRTFLLKYN	0.8685	Strong binder
DRB1_0101	QTYVTQQLIRAAEIR	0.8673	Strong binder
DRB1_0101	TGRLQSLQTYVTQQL	0.8638	Strong binder
DRB1_0101	AYYVGYLQPRTFLLK	0.8627	Strong binder
DRB1_0101	SLQTYVTQQLIRAAE	0.8532	Strong binder
DRB1_0101	IIAYTMSLGAENSV	0.8529	Strong binder
DRB1_0101	ITGRLQSLQTYVTQQ	0.8523	Strong binder
DRB1_0101	GWTFGAGAALQIPFA	0.8445	Strong binder
DRB1_0101	IAYTMSLGAENSVAY	0.8429	Strong binder
DRB1_0101	FELLHAPATVCGPKK	0.8406	Strong binder
DRB1_0101	VGYLQPRTFLLKYNE	0.8399	Strong binder
DRB1_0101	GRLQSLQTYVTQQLI	0.8386	Strong binder
DRB1_0101	QSLQTYVTQQLIRAA	0.8351	Strong binder
DRB1_0101	LNTLVKQLSSNFGAI	0.8337	Strong binder
DRB1_0101	WTFGAGAALQIPFAM	0.8331	Strong binder
DRB1_0101	SIIAYTMSLGAENSV	0.8331	Strong binder
DRB1_0101	NLTLVKQLSSNFGAIS	0.8330	Strong binder
DRB1_0101	LITGRLQSLQTYVTQ	0.8329	Strong binder
DRB1_0101	RVVLSFELLHAPAT	0.8315	Strong binder
DRB1_0101	SSNFGAISSVLNDIL	0.8297	Strong binder
DRB1_0101	AAYVGYLQPRTFLL	0.8264	Strong binder
DRB1_0101	GKGYHLMSFPQSAPH	0.8264	Strong binder
DRB1_0101	SGWTFGAGAALQIPF	0.8240	Strong binder
DRB1_0101	KGYHLMSFPQSAPHG	0.8223	Strong binder
DRB1_0101	TYVTQQLIRAAEIRA	0.8219	Strong binder
DRB1_0101	AQKFNGLTVLPPLLT	0.8195	Strong binder
DRB1_0101	QIPFAMQMAYRFNGI	0.8164	Strong binder
DRB1_0101	LSSNFGAISSVLNDI	0.8149	Strong binder
DRB1_0101	TRFQTLALHRSYLT	0.8132	Strong binder
DRB1_0101	AYTMSLGAENSVAYS	0.8128	Strong binder
DRB1_0101	NFNFNGLTGTGVLTE	0.8104	Strong binder
DRB1_0101	ALNTLVKQLSSNFGA	0.8094	Strong binder
DRB1_0101	CGKGYHLMSFPQSAP	0.8087	Strong binder
DRB1_0101	QKFNGLTVLPPLTD	0.8084	Strong binder
DRB1_0101	SNFGAISSVLNDILS	0.8082	Strong binder
DRB1_0101	LQIPFAMQMAYRFNG	0.8069	Strong binder
DRB1_0101	VNFNFNGLTGTGVLT	0.8064	Strong binder
DRB1_0101	TLVKQLSSNFGAISS	0.8047	Strong binder
DRB1_0101	TSGWTFGAGAALQIP	0.8027	Strong binder